Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

946-30-5 | DTXSID4061339

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.14e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.33e-01

Confidence level: 3.63e-01

Nearest Neighbors from the Training Set

Image not found
2-Ethylhexyl diphenyl phosphate
Measured: 3.00e-10
Predicted: 1.52e-05

Image not found
3,5-Dichlorodiphenyl ether
Measured: 3.45e-06
Predicted: 9.56e-04

Image not found
Tetrakis(trimethylsiloxy)silane
Measured: 7.50e-10
Predicted: 8.27e-02

Image not found
Pyrazoxyfen
Measured: 2.25e-09
Predicted: 8.53e-08